Comparison of x-ray formfactors determined by SAXS experiments and MD-simulation

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Formfactors of DCOP/DPPC/CHOL and DOPC/DSPC/CHOL lipid mixtures

Here we compare x-ray formfactors (FF) obtained from diffraction patterns of multilamellar vesicles (MLV) containing DCOP/DPPC/CHOL and DOPC/DSPC/CHOL with formfactors obtained by MD-simulations (Figs. 1, 2). Exact lipid compositions for SAXS experiments and MD-simulations are listed in Table 1. Bilayer thicknesses (distance between phosphate groups(PCN)) determined by SAXS and MD-simulations are summarized in Table 2.

Table 1: Lipid compositions (molar fractions) of measured samples. Same lipid compositions were used for SAXS experiments and MD-simulations. DOPC/DPPC/CHOL system was measured at $T = 15\,℃$ and DOPC/DSPC/CHOL was measured at $T = 22\,℃$

	phase	DOPC	DPPC	DSPC	CHOL
DOPC/DPPC/CHOL	L_d	0.66	0.19	0.0	0.15
	L_o	0.12	0.58	0.0	0.3
DOPC/DSPC/CHOL	L_d	0.74	0.0	0.09	0.17
	L_o	0.12	0.0	0.56	0.32

Table 2: Bailyer thickness (d_B) of measured samples.

	d_B SAXS [Å]	d_B MD-Sim [Å]
DOPC/DPPC/CHOL - L_d	40.8 ± 0.8	42.7
DOPC/DPPC/CHOL - L_o	47.9 ± 0.9	48.2
DOPC/DSPC/CHOL - L_d	40.6 ± 0.8	42.4
DOPC/DSPC/CHOL - L_o	51.2 ± 1.0	50.9

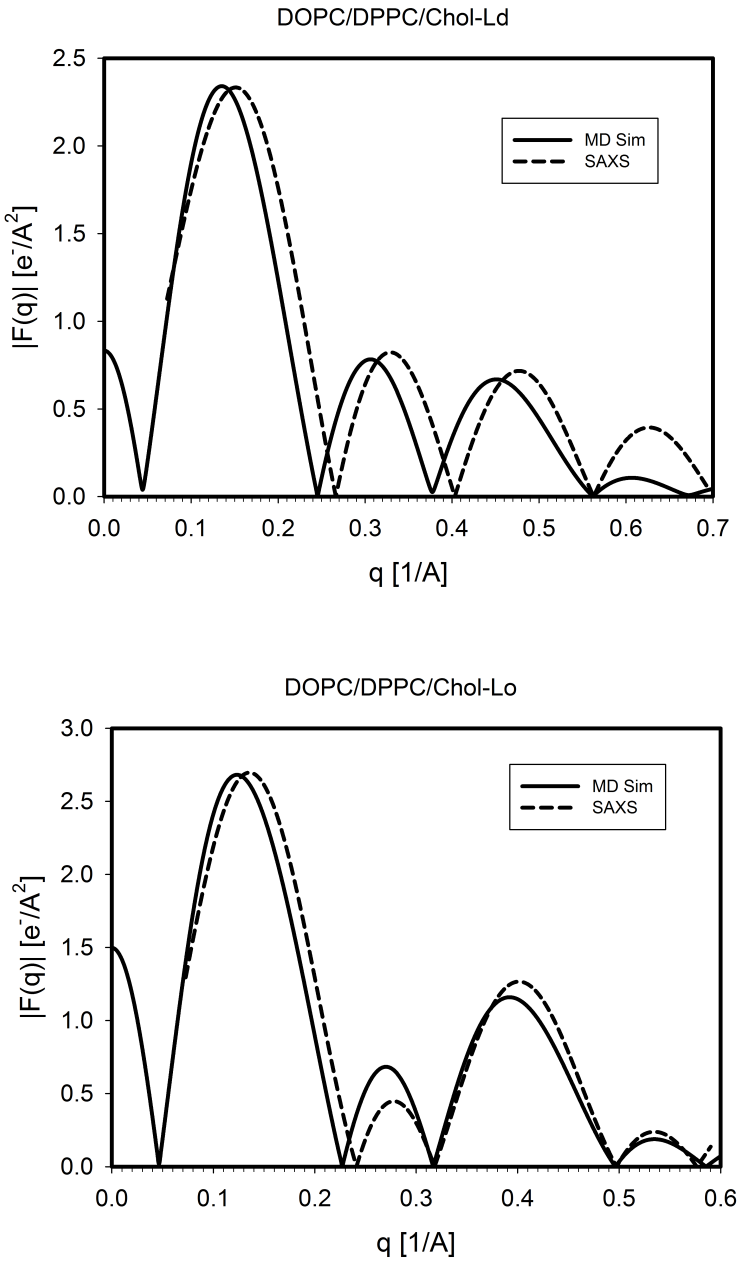

Figure 1: Comparison of x-ray formfactors determined by MD-simulations (solid line) and by SAXS experiments (dashed line). Amplitude of the experimental FF was normalized to simulated FF for comparison.

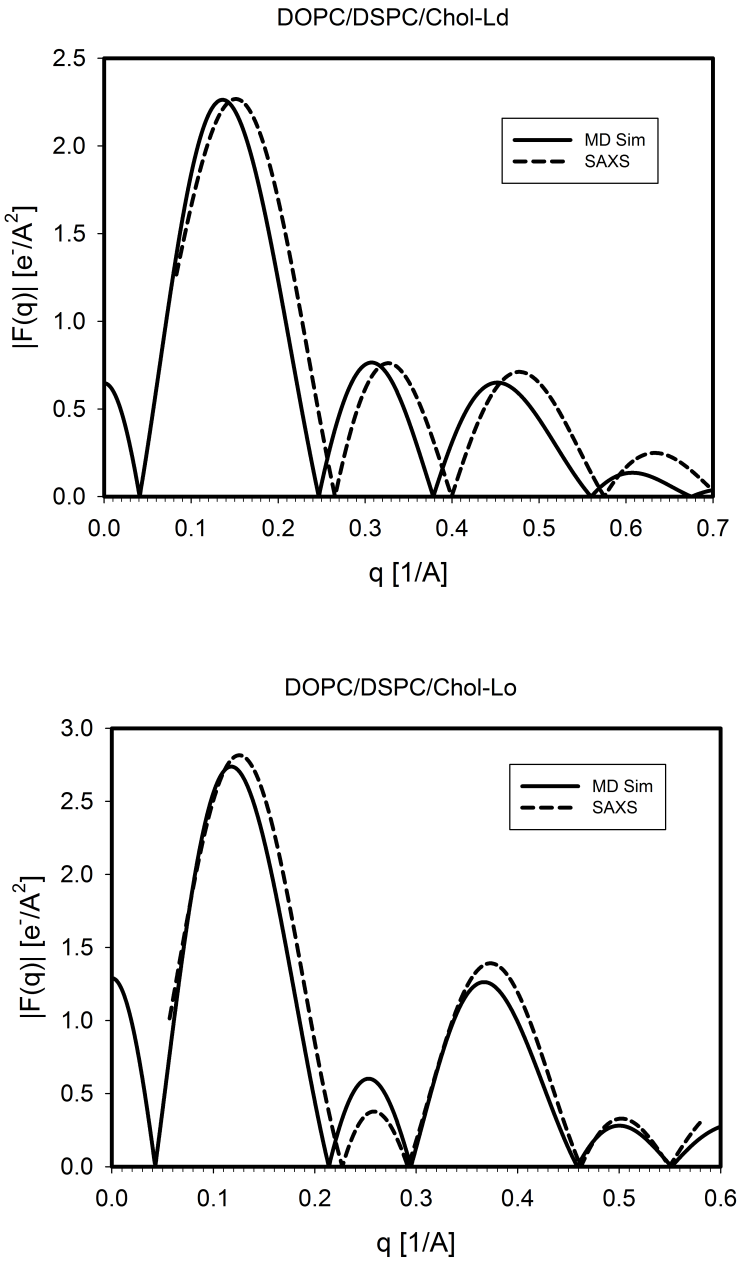

Figure 2: Comparison of x-ray formfactors determined by MD-simulations (solid line) and by SAXS experiments (dashed line). Amplitude of the experimental FF was normalized to simulated FF for comparison.

Fitting of experimental SAXS data

We also checked if it is possible to fit the experimental data with the formfactor that we obtained by MD-simulation. Therefore we used the simulated FF and combined it with the structure factor of the Caille Theory, that we are using for our fitting routine. As it is shown in Figs. 3 and 5 the simulated FF acnnot describe the experimental data of the L_d phases most of all because the minima of the simulated FF are at to low q-values. Figs. 4 and 6 are representing the experimental data and model fits of L_o phase samples. The minima of the simulated FFs are at similar positions as the minima of the experimentally determined FFs and therefore it is somehow possible to fit the experimental data with the simulated FFs.

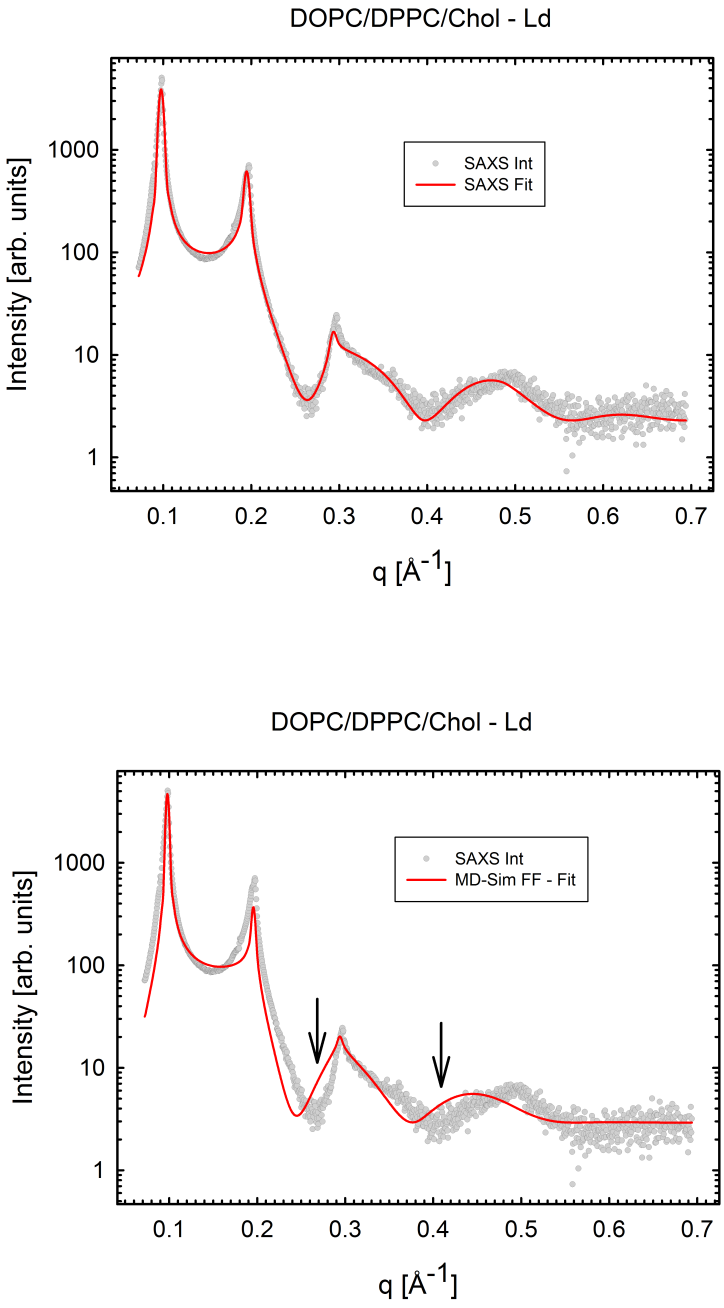

Figure 3: Model fits to experimental SAXS data. Upper panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line). Lower panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line) with the simulated FF that was fixed within the fitting procedure.

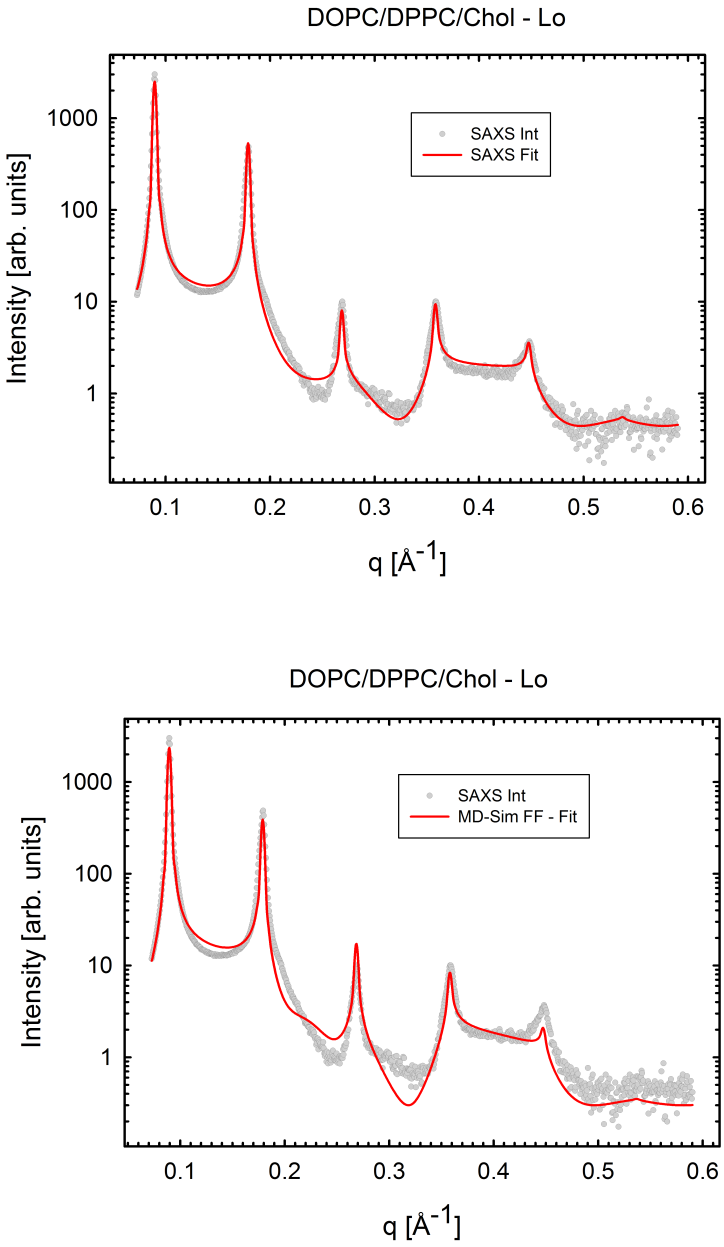

Figure 4: Model fits to experimental SAXS data. Upper panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line). Lower panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line) with the simulated FF that was fixed within the fitting procedure.

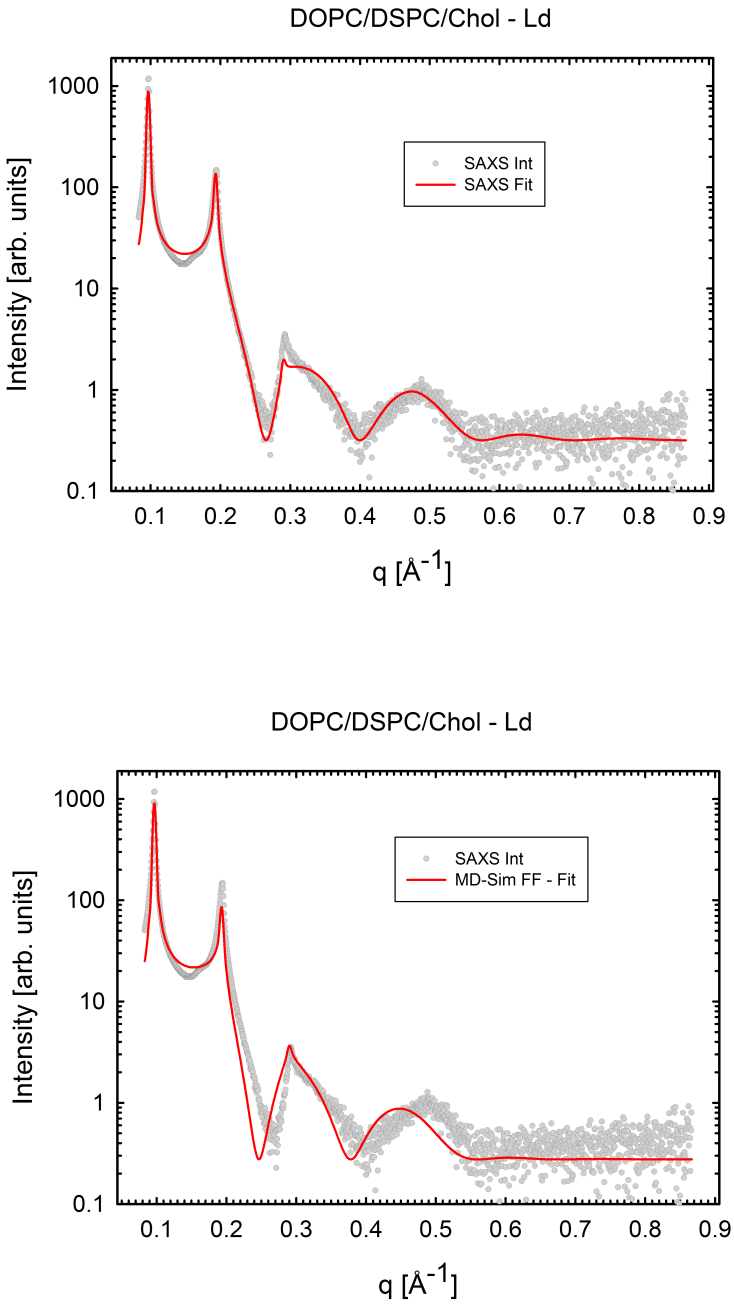

Figure 5: Model fits to experimental SAXS data. Upper panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line). Lower panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line) with the simulated FF that was fixed within the fitting procedure.

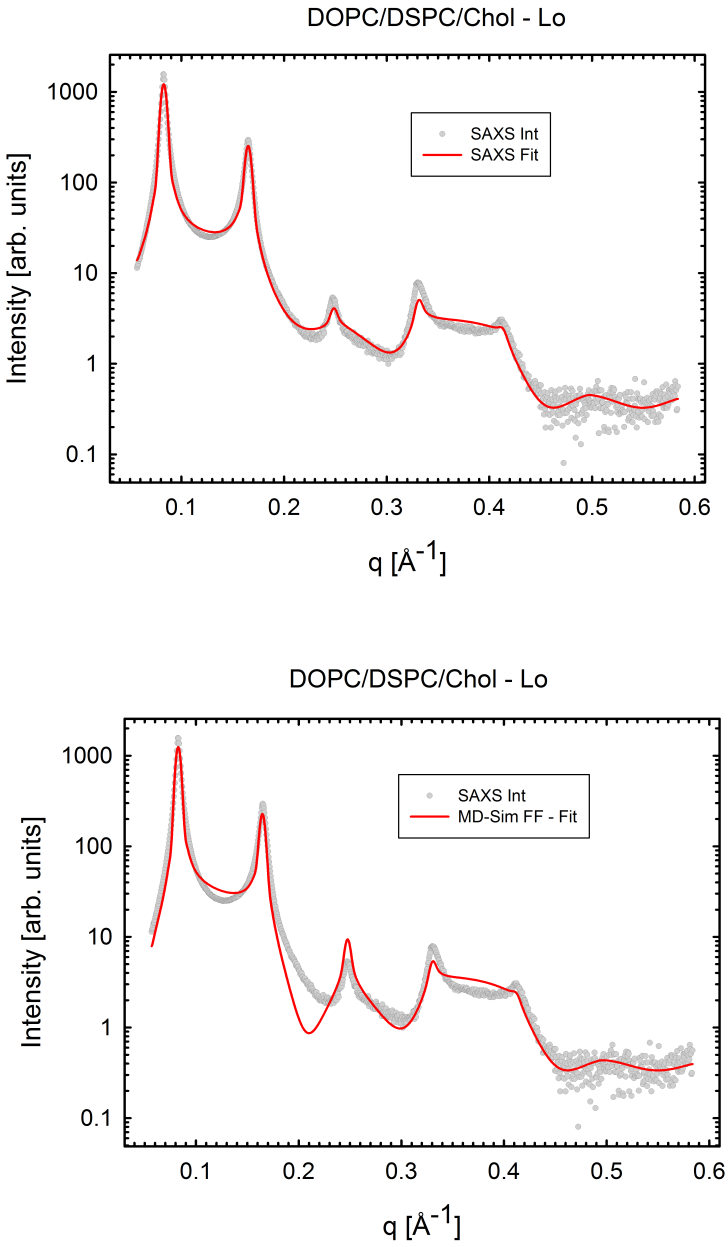

Figure 6: Model fits to experimental SAXS data. Upper panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line). Lower panel shows experimental SAXS dadta (gray circles) and the corresponding model fit (red line) with the simulated FF that was fixed within the fitting procedure.